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GENERAL TOPOLOGICAL INDICES OF CIRCUMCORONENE SERIES OF BENZENOID

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ABSTRACT

In this paper, we determine generalized version of the first Zagreb index, general connectivity index, general sum connectivity index, general reformulated index and other topological indices for circumcoronene series of benzenoid.

Keywords: *Zagreb indices, connectivity index, sum connectivity index, reformulated index, K-edge index, circumcoronene series of benzenoid.*

Mathematics Subject Classification: *05CO5.*

1. INTRODUCTION

The graphs considered here are finite, undirected without loops and multiple edges. Let G be a connected graph. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge e in G, which is defined by $d_G(e) = d_G(u) + d_G(v) – 2$ with $e = uv$. For all further notation and terminology we refer to reader to [1].

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These indices are useful for establishing correlation between the structure of a molecular compound and its physico-chemical properties.

The first and second Zagreb indices of a graph G are defined as

$$M_1(G)=\sum_{u\in V(G)} d_G(u)^2 \qquad \text{or} \qquad M_1(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right]$$

$$M_2(G)=\sum_{uv\in E(G)} d_G(u)d_G(v).$$

These indices were introduced by Gutman *et al.* in [2].

Another vertex degree based topological index was defined in [2] and it was studied by Furtula *et al.* in [3].

The forgotten topological index or F-index is defined as

$$F(G)=\sum_{u\in V(G)} d_G(u)^3.$$

The generalized version of the first Zagreb index [4] of a graph G is defined as

$$M_1^{a+1}(G)=\sum_{u\in V(G)} d_G(u)^{a+1}=\sum_{uv\in E(G)}\left[d_G(u)^a+d_G(v)^a\right], \text{ where } a\in R. \tag{1}$$

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The modified first and second Zagreb indices [5] are respectively defined as

$$ {}^{m}M_1(G)=\sum_{u\in V(G)}\frac{1}{d_G(u)^2}, \qquad {}^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d_G(u)d_G(v)}. $$

The first hyper-Zagreb index of a graph G is defined as

$$ HM_1(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right]^2. $$

This index was introduced by Shirdel *et al.* in [6].

The sum connectivity index of a graph G is defined as

$$ X(G)=\sum_{uv\in E(G)}\sqrt{\frac{1}{d_G(u)+d_G(u)}} $$

This index was introduced by Zhou and Trinajstić in [7].

The general sum connectivity index was introduced by Zhou and Trinajstić in [8] and it is defined as

$$ M_1^a(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)\right]^a. \tag{2} $$

This index was also studied, for example, in [9].

In [10], the second hyper Zagreb index of a graph G is defined as

$$ HM_2(G)=\sum_{uv\in E(G)}\left[d_G(u)d_G(v)\right]^2. $$

The Randić index or product connectivity index of a graph G is defined as

$$ \chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)d_G(v)}}. $$

This topological index was proposed by Randić in [11] and was studied, for example, in [12, 13].

The general product connectivity index [9, 14] is defined as

$$ M_2^a(G)=\sum_{uv\in E(G)}\left[d_G(u)d_G(v)\right]^a \tag{3} $$

The reformulated first Zagreb index of a graph G is defined as

$$ EM_1(G)=\sum_{e\in E(G)}d_G(e)^2. $$

This index was introduced by Miličević *et al.* in [15].

Recently in [16], Kulli introduced the K-edge index of a graph G and it is defined as

$$ K_e(G)=\sum_{e\in E(G)}d(e)^3. $$

This index was also studied in [17].

The general reformulated Zageb index [18] of a graph G is defined as

$$ EM_1^a(G)=\sum_{e\in E(G)}d(e)^a \tag{4} $$

where a is a real number.

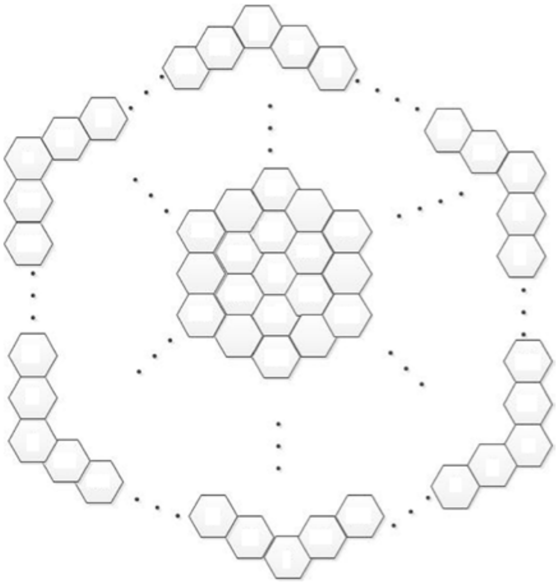

Figure-1: The graph of circumcoronene series of benzenoid H_k, $k \geq 1$.

In this paper, we compute several topological indices for cirumcoronene series of benzenoid H_k, $k \geq 1$.

The benzene molecule is a molecule in chemistry and nanosciences and it is useful to synthesize aromatic compounds. The circumcoronene series of benzenoid is a benzenoid family and it is symbolized by H_k, $k \geq 1$ which consists copies of benzene C_6 on circumference, see [19].

By algebraic method, we obtain $|V(H_k)| = 6k^2$ and $|E(H_k)| = 9k^2 - 3k$. From Figure 1, it is easy to see that there are two partitions of the vertex set of H_k as follows:

$$V_2 = \{u \in V(H_k) \mid d_{H_k}(u) = 2\},\ |V_2| = 6k.$$

$$V_3 = \{u \in V(H_k) \mid d_{H_k}(u) = 3\},\ |V_3| = 6k(k-1).$$

Also by algebraic method, we obtain three edge partitions of H_k based on the sum of degrees of the end vertices as follows:

$$E_4 = E_4^* = \{uv \in E(H_k) \mid d_{H_k}(u) = d_{H_k}(v) = 2\},\ |E_4| = |E_4^*| = 6.$$

$$E_5 = E_6^* = \{uv \in E(H_k) \mid d_{H_k}(u) = 2, d_{H_k}(v) = 3\},\ |E_5| = |E_6^*| = 12(k-1)$$

$$E_6 = E_9^* = \{uv \in E(H_k) \mid d_{H_k}(u) = d_{H_k}(v) = 3\},\ |E_6| = |E_9^*| = 9k^2 - 15k + 6.$$

The edge degree partition of H_k is given in Table 1.

$d_{H_k}(u), d_{H_k}(v) \backslash e = uv \in E(H_k)$	(2, 2)	(2, 3)	(3,3)
$d_{H_k}(e)$	2	3	4
Number of edges	6	$12(k-1)$	$9k^2-15k+6$

Table-1: Edge degree partition of H_k

We compute the generalized version of the first Zagreb index of H_k.

Theorem 1: The generalized version of the first Zagreb index of H_k is given by

$$M_1^{a+1}(H_k) = \left(3^{a+1}\right)6k^2 + \left(2^{a+1} - 3^{a+1}\right)6k. \tag{5}$$

Proof: Let $G = H_k$. From equation (1) and by cardinalities of the vertex partition of H_k, we have

$$M_1^{a+1}(H_k) = \sum_{u \in V(H_k)} d(u)^{a+1} = \sum_{u \in V_2} d(u)^{a+1} + \sum_{u \in V_3} d(u)^{a+1}$$

$$= 2^{a+1}6k + 3^{a+1}6k(k-1) = \left(3^{a+1}\right)6k^2 + \left(2^{a+1} - 3^{a+1}\right)6k.$$

We obtain the following corollaries by using Theorem 1.

Corollary 1.1: The first Zagreb index of H_k is given by $M_1(H_k) = 54k^2 - 30k$.

Proof: Put $a = 1$ in equation (5), we obtain the desired result.

Corollary 1.2: The F-index of H_k is given by $F(H_k) = 162k^2 - 114k$.

Proof: Put $a = 2$ in equation (5), we obtain the desired result.

Corollary 1.3: The modified first Zagreb index of H_k is given by ${}^{m}M_1(H_k) = \frac{2}{3}k^2 + \frac{5}{36}k$.

Proof: Put $a = -3$ in equation (5), we obtain the desired result.

In the next result, we determine the general sum connectivity index of H_k, $k \geq 1$.

Theorem 2: The general sum connectivity index of H_k is given by

$$M_1^a(H_k) = 9 \times 6^a k^2 + \left(4 \times 5^a - 5 \times 6^a\right)3k + \left(4^a - 2 \times 5^a + 6^a\right)6 \tag{6}$$

Proof: From equation (2) and cardinalities of the edge partitions of H_k, we have

$$M_1^a(H_k) = \sum_{uv \in E(H_k)} \left[d_{H_k}(u) + d_{H_k}(v)\right]^a$$

$$= \sum_{uv \in E_4} \left[d_{H_k}(u) + d_{H_k}(v)\right]^a + \sum_{uv \in E_5} \left[d_{H_k}(u) + d_{H_k}(v)\right]^a + \sum_{uv \in E_6} \left[d_{H_k}(u) + d_{H_k}(v)\right]^a$$

$$= 4^a \times 6 + 5^a \times 12(k-1) + 6^a \times \left(9k^2 - 12k + 6\right)$$

$$= 9 \times 6^a k^2 + \left(4 \times 5^a - 5 \times 6^a\right)3k + \left(4^a - 2 \times 5^a + 6^a\right)6$$

We obtain the following corollaries by using Theorem 2.

Corollary 2.1: The first Zagreb index of H_k is given by $M_1(H_k) = 54k^2 - 30k$.

Proof: Put $a = 1$ in equation (6), we get the desired result.

Corollary 2.2: The first hyper-Zagreb index of H_k is given by $HM_1(H_k) = 324k^2 - 240k + 12$.

Proof: Put $a = 2$ in equation (6), we get the desired result.

Corollary 2.3: The sum connectivity index of H_k is given by $X(H_k) = \frac{1}{10}(15k^2 - k + 1)$.

Proof: Put $a = -\frac{1}{2}$ in equation (6), we get the desired result.

We now compute the general product connectivity index of H_k, $k \geq 1$.

Theorem 3: The general product connectivity index of H_k is given by

$$M_2^a(H_k) = 9^{a+1}k^2 + \left(12 \times 6^a - 15 \times 9^a\right)k + \left(6 \times 4^a - 12 \times 6^a + 6 \times 9^a\right). \tag{7}$$

Proof: From equation (3) and by cardinalities of the edge partition of H_k based on the product degrees of the end vertices, we have

$$M_2^a(H_k) = \sum_{uv \in E(H_k)} \left[d_{H_k}(u) d_{H_k}(v)\right]^a$$

$$= \sum_{uv \in E_4} \left[d_{H_k}(u) d_{H_k}(v)\right]^a + \sum_{uv \in E_5} \left[d_{H_k}(u) d_{H_k}(v)\right]^a + \sum_{uv \in E_6} \left[d_{H_k}(u) d_{H_k}(v)\right]^a$$

$$= 4^a \times 6 + 6^a \times 12(k-1) + 9^a \times \left(9k^2 - 15k + 6\right)$$

$$= 9^{a+1}k^2 + \left(12 \times 6^a - 15 \times 9^a\right)k + \left(6 \times 4^a - 12 \times 6^a + 6 \times 9^a\right).$$

We obtain the following corollaries by Theorem 3.

Corollary 3.1: The second Zagreb index of H_k is given by $M_2(H_k) = 81k^2 - 63k + 6$.

Proof: Put $a = 1$ in equation (7), we get the desired result.

Corollary 3.2: The second hyper Zagreb index of H_k is given by
$HM_2(H_k) = 729k^2 - 783k + 150$.

Proof: Put $a = 2$ in equation (7), we get the desired result.

Corollary 3.3: The modified second Zagreb index of H_k is given by ${}^mM_2(H_k) = k^2 + \frac{1}{3}k + \frac{1}{6}$.

Proof: Put $a = -1$ in equation (7), we get the desired result.

Corollary 3.4: The Randić connectivity index of H_k is given by $\chi(H_k) = 3k^2 + \left(2\sqrt{6} - 5\right)\left(k - 1\right)$

Proof: Put $a = -\frac{1}{2}$ in equation (7), we get the desired result.

In the following theorem, we compute the general first reformulated Zagreb index of H_k, $k \geq 1$.

Theorem 4: The general first reformulated Zagreb index of H_k is given by

$$EM_1^a(H_k) = 9 \times 4^a k^2 + \left(12 \times 3^a - 15 \times 4^a\right)k + \left(6 \times 2^a - 12 \times 3^a + 6 \times 4^a\right). \tag{8}$$

Proof: From equation (4) and by the edge degree partition of H_k, we have

$$\begin{aligned} EM_1^a(H_k) &= \sum_{e \in E(G)} d_G(e)^a = \sum_{e \in E_4} d_G(e)^a + \sum_{e \in E_5} d_G(e)^a + \sum_{e \in E_6} d_G(e)^a \\ &= 6 \times 2^a + 12(k-1) \times 3^a + \left(9k^2 - 15k + 6\right) \times 4^a \\ &= 9 \times 4^a k^2 + \left(12 \times 3^a - 15 \times 4^a\right)k + \left(6 \times 2^a - 12 \times 3^a + 6 \times 4^a\right). \end{aligned}$$

We obtain the following results by using Theorem 4.

Corollary 4.1: The first reformulated Zagreb index of H_k is given by $EM_1(H_k) = 144k^2 - 132k + 12$.

Proof: Put $a = 2$ in equation (8), we get the desired result.

Corollary 4.2: The K-edge index of H_k is given by $K_e(H_k) = 576k^2 - 636k + 108$.

Proof: Put $a = 3$ in equation (8), we get the desired result.

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